# ROOM TEMPERATURE GAS-PHASE GIBBS ENERGIES OF WATER AMINE COMPLEXES

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A hydrogen bound bimolecular complex consists of a hydrogen bond donor and acceptor unit. The OH-stretching fundamental transition of the hydrogen bond donor is typically redshifted and its infrared intensity enhanced upon complexation.[1] This facilitates detection of weak complexes even though the equilibrium is strongly shifted towards the monomers at room temperature. The ratio of a measured and calculated intensity of a vibrational band is proportional to the complex abundance, which with known monomer pressures gives the equilibrium constant.[2] We calculate absolute transition intensities with a reduced dimensionality variational local mode model that also includes low-frequency vibrations. Calculated and experimental intensities of multiple bands are combined to give the equilibrium constant of complex formation for the water·dimethylamine and water·trimethylamine complex.[3] The equilibrium constant obtained from different bands should be equivalent, and the detection of multiple bands therefore allows us to validate the accuracy of our combined experimental and theoretical approach.

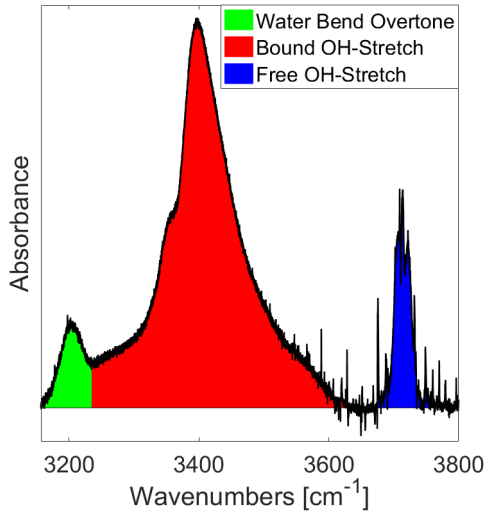


Figure 1: Room temperature gas-phase infrared spectrum of the water·dimethylamine complex.

[1] Arunan, Elangannan, et al. Pure Appl. Chem., 2011, **83.8**, 1619.
[2] A. S. Hansen, E. Vogt, and H. G. Kjaergaard, Int. Rev. Phys. Chem., 2019, **38.1**, 115.
[3] A. Kjaersgaard, E. Vogt, A. S. Hansen, and H. G. Kjaergaard, J. Phys. Chem. A., 2020, **124.35**, 7113.